

## REMARKS

### I. Status of the claims

Claims 1-4, 7-16, 20-27, and 30-44 are pending. Claims 39-44 have been withdrawn and claims 5, 6, 17-19, 28, and 29 have been cancelled. In this response, claims 1-4, 7-9, 16, 20, 21, 24, 25, 27, and 30-32 have been amended.

Various features have been introduced into independent claims 1, 16, and 27. First, the claims have been amended to be directed to a method of calculating an intermolecular interaction energy, and the steps of determining an interaction energy and calculating an intermolecular interaction energy, such as those originally recited in claims 5 and 6, have been incorporated into the independent claims. Second, the claims have been amended to better clarify that a cap member is introduced at each decomposition point in the molecular fragment. Support for this amendment may be found in paragraphs 38-40 of the specification. Third, the claims have been amended to better clarify the role of the conjugate caps. In particular, the step of coupling the caps and determining the interaction action between the conjugated caps and the second molecule has been introduced. Support for these amendments may be found in paragraphs 64 and throughout the specification. Fourth, the claims have been amended to recite that the results of the calculated intermolecular interaction energy are displayed. Support for this amendment may be found in Figs. 6-10 and 12 and their corresponding description in paragraphs 17-23 and 69-75. Other amendments have been made to dependent claims 2-4, 7-9, 20, 21, 24, 25, and 30-32 to more clearly recite the claimed subject matter. No new matter has been introduced through these amendments.

Applicants' representatives conducted a telephonic interview with Examiner Moran on July 11, 2007 to discuss the Office Action. Proposed amendments to claims 1 and 2 were provided to the examiner. The rejection under 35 U.S.C. § 101 and the rejections relating to the conjugate caps were discussed, with the examiner providing Applicants with helpful comments relating to those rejections. Applicants thank the examiner for her time and assistance in providing the interview.

### II. Objections to specification

The examiner has objected to pages 6, 11, and 14 in the specification as containing an

embedded hyperlink and/or browser-executable code. In this response, Applicants have amended paragraphs 27, 44, and 53 to remove the objected-to links.

III. Rejection under 35 U.S.C. § 101

The examiner has rejected claims 1-38 under 35 U.S.C. § 101 because the claimed invention is alleged directed to non-statutory subject matter.

This rejection was discussed in the interview, with the examiner emphasizing that the claims should recite a concrete, tangible, and useful result. An example of concrete, tangible, and useful result may be seen in the displaying of calculations in the graphs shown in Figs. 6-10 and 12. In view of the disclosure, the examiner suggested that a claim element reciting that the calculations were displayed would overcome this rejection.

In this response, Applicants have added display steps to each of the independent claims, per the examiner's suggestion. Applicants have further amended claim 16 to recite that the computer-readable medium is a physical medium and further amended claim 27 to recite that system is a computer system to emphasize the tangible features of the claims.

In view of these amendments, Applicants respectfully request that the examiner withdraw the rejections under 35 U.S.C. § 101.

IV. Rejections under 35 U.S.C. § 112 relating to conjugate caps

The examiner has rejected claims 1-38 under 35 U.S.C. § 112, first paragraph as failing to comply with the written description requirement, and under 35 U.S.C. § 112, second paragraph as failing to particularly point out and distinctly claim the invention.

Both rejections relate to the term "conjugate caps" recited in claimed invention. As explained in the interview, a cap member is introduced at each decomposition point in the molecular fragment. The caps preserve the valence of the bond being cut and, preferably, mimic the effect of the of the original molecular part being cut away from the remaining fragment. See paragraph 40 of the specification. For instance, for the molecule shown in Fig. 1, one skilled in the art may add the cap  $\text{NH}_2$  on to the A2 molecular fragment at the left decomposition point to mimic the nA1 portion. Other caps that similar mimic the removed portion may be used.

When performing intermolecular interaction energy calculations, the added caps should be factored in the calculations. To account for the caps, they can be coupled together and their interaction energy between the caps and the second molecule can be determined. Preferably, the interaction energy of caps is subtracted from the interaction energy determined between the first molecule and the second molecule. This provides a better and more accurate determination of the intermolecular interaction energy between the first molecule and the second molecule.

To better claim the function of the conjugate caps, Applicants have introduced amendments into the claims to show that the caps are coupled and then used to calculate an interaction energy. The interaction energy determined between the conjugated caps and the second molecule is used when calculating the intermolecular interaction energy between the first molecule and second molecule. Applicants have also amended the claims to avoid any confusion relating to the term “conjugate” when discussing the caps that are introduced onto the molecular fragments.

These amendments clarify the role of the caps, as supported by the specification. See, in particular, paragraph 64, discussing the coupling of the caps and their use to determine interaction energies. Accordingly, Applicants respectfully request that the examiner withdraw the rejections under 35 U.S.C. § 112, first paragraph and the rejections under 35 U.S.C. § 112, second paragraph relating to the term “conjugate caps.”

V. Rejection of claims 1, 16, and 27 under 35 U.S.C. § 112, second paragraph

The examiner has rejected claims 1, 16, and 27 under 35 U.S.C. § 112, second paragraph because of the alleged lack of clarity relating to the phrase “at one or more locations in the molecule.” In this response, Applicants have replaced that phrase with the phrase “at each decomposition point in the molecular fragment.” The amended phrase, when read in conjunction with the rest of claim, more clearly demonstrates that a cap is introduced on to a molecular fragment to create a molecular portion. Accordingly, Applicants respectfully request that this rejection be withdrawn.

VI. Rejection of claim 7 under 35 U.S.C. § 112, second paragraph

The examiner has rejected claim 7 under 35 U.S.C. § 112, second paragraph because of

the alleged lack of clarity relating to the term “computing systems.” In this response, Applicants have amended claim 7 by rewording the placement of the computing-systems terms in the claims to clarify that the method *calculates* an interaction energy *on* a computing system. In view of this clarifying amendment, Applicants respectfully request that the examiner withdraw this rejection under 35 U.S.C. § 112, second paragraph.

VII. Conclusion

Except for issue fees payable under 37 C.F.R. §1.18, the Commissioner is hereby authorized by this paper to charge any additional fees during the entire pendency of this application including fees due under 37 C.F.R. §§1.16 and 1.17 which may be required, including any required extension of time fees, or credit any overpayment to Deposit Account No. 19-2380. This paragraph is intended to be a **CONSTRUCTIVE PETITION FOR EXTENSION OF TIME** in accordance with 37 C.F.R. §1.136(a)(3).

Respectfully submitted,

/Jeffrey N. Townes, Reg. No. 47,142/  
Jeffrey N. Townes  
Registration No. 47,142

Dated: July 23, 2007

**Customer No. 22204**  
NIXON PEABODY LLP  
Suite 900, 401 9<sup>th</sup> Street, N.W.  
Washington, D.C. 20004-2128  
202.585.8000